

Kato's inequality and asymptotic spectral properties for discrete magnetic Laplacians

Józef Dodziuk and Varghese Mathai

ABSTRACT. In this paper, a discrete form of the Kato inequality for discrete magnetic Laplacians on graphs is used to study asymptotic properties of the spectrum of discrete magnetic Schrödinger operators. We use the existence of a ground state with suitable properties for the ordinary combinatorial Laplacian and semigroup domination to relate the combinatorial Laplacian with the discrete magnetic Laplacian. Our techniques yield existence and uniqueness of the fundamental solution for the heat kernel on a graph of bounded valence.

Introduction

The discrete magnetic Laplacian (DML), Δ_σ and discrete magnetic Schrödinger operator (DMSO), $\Delta_\sigma + T$, where T is in the commutant of a projective G action, on graphs had been studied for many years by condensed matter and solid state physicists, mainly on graphs having a free action of a crystallographic group G cf. [2]. In particular, these operators are Hamiltonians for the discrete model of the quantum Hall effect. Sunada [14] extended the definition of these operators to arbitrary graphs equipped with a free action of a general finitely generated discrete group G .

In this paper, we establish asymptotic properties of the spectrum of DMLs and DMSOs, such as the large time decay of the G -trace of the heat kernels of these operators, and also the positivity of the Fuglede-Kadison determinant of these operators - these results could have applications to physics, particularly to analysis of the fractional quantum Hall effect.

A discrete form of the Kato inequality is used in the paper. Other applications of it are in [16], for finite graphs and by physicists in the case of graphs having a free action of a crystallographic group. Together with semigroup domination techniques and some well known results of Varopoulos [17], the desired asymptotic properties of the spectrum of DMLs and DMSOs of the form $\Delta_\sigma + T$, where $T \geq 0$ is established here. This result is optimal in the case when G is amenable - here the characterization of amenability of G via the bottom of the spectrum of the discrete Laplacian λ_0 due to R. Brooks [4], [15] is used. In the nonamenable case, we establish basic properties of the ground state of the discrete

Laplacian, and use it to establish asymptotic properties of the spectrum of DMSOs of the form $\Delta_\sigma + T$, where $T \geq -\lambda_0$.

1. Kato's inequality

We show that the technique of domination of semigroups as developed in [9] can be used to relate discrete magnetic Laplacians on a graph with the ordinary discrete Laplacian. Our proofs follow closely [3]. We begin with the positivity preserving property of the ordinary discrete Laplacian

$$\Delta : C_{(2)}^0(K) \longrightarrow C_{(2)}^0(K)$$

acting on the space of square-integrable cochains on the graph K , i.e. the space of complex-valued functions f on vertices of K such that $\sum_v |f(v)|^2 < \infty$. For a function $f \in C_{(2)}^0(K)$ and a vertex v of K

$$(1) \quad \Delta f(v) = \sum_{w \sim v} (f(v) - f(w))$$

where the notation $w \sim v$ denotes that v and w are connected by an edge.

LEMMA 1.1. *Suppose $f \in C_{(2)}^0(K)$ is a real-valued function and $\lambda > 0$. If $(\Delta + \lambda I)f \geq 0$, then $f \geq 0$ i.e. $(\Delta + \lambda I)^{-1}$ is positivity preserving.*

PROOF. Suppose f satisfies the assumptions of the lemma but attains a negative value. Since $f \in C_{(2)}^0(K)$ it vanishes at infinity and therefore attains a negative minimum at a vertex v_0 of K . Now, by (1)

$$(\Delta + \lambda I)f(v_0) = \sum_{w \sim v_0} (f(v_0) - f(w)) + \lambda f(v_0).$$

The left-hand side of this equality is nonnegative by assumption whereas the right-hand side is strictly negative. The contradiction proves the lemma. \square

Now let Δ_σ be the discrete magnetic Laplacian (DML) associated to a multiplier function σ with values in $U(1)$. In particular, σ is a function defined on oriented edges of K and satisfies $\sigma([u, v]) = \overline{\sigma([v, u])}$. Explicitly,

$$(2) \quad \Delta_\sigma f(v) = \sum_{w \sim v} (f(v) - \sigma([w, v])f(w)).$$

Our analog of Kato's inequality is as follows.

LEMMA 1.2. *For every $f \in C_{(2)}^0(K)$, one has the pointwise inequality:*

$$|f| \cdot \Delta|f| \leq \Re(\Delta_\sigma f \cdot \overline{f}).$$

PROOF. By an explicit calculation using (1) and (2),

$$(|f| \cdot \Delta|f|)(v) - \Re(\Delta_\sigma f \cdot \overline{f})(v) = \sum_{w \sim v} \Re(\sigma([w, v])f(w)\overline{f(v)}) - |f(v)| \cdot |f(w)| \leq 0.$$

\square

Recall that the bottom of the spectrum of a self-adjoint operator such as the DML is computed as:

$$\lambda_0(\Delta_\sigma) = \inf \left\{ \frac{(\Delta_\sigma f, f)}{\|f\|^2} : \|f\| \neq 0 \right\}$$

where $\|f\|$ denotes the ℓ^2 -norm of $f \in C_{(2)}^0(K)$ and $(\Delta_\sigma f, f)$ the ℓ^2 -inner product. As an immediate corollary of Lemma 1.2, one has,

COROLLARY 1.3. *On $C_{(2)}^0(K)$, one has the inequality*

$$\lambda_0(\Delta) \leq \lambda_0(\Delta_\sigma).$$

Recall the theorem of Kesten and Brooks [4], which says that for finitely generated, infinite groups, one has $\lambda_0(\Delta) = 0$ if and only if G is an amenable group. The following is an immediate corollary of this fact and Corollary 1.3.

COROLLARY 1.4. *If G is a nonamenable group, then on $C_{(2)}^0(K)$, one has*

$$\lambda_0(\Delta_\sigma) > 0.$$

Note that we regard $C_{(2)}^0(K)$ as a Hilbert space with the inner product

$$(f, g) = \sum_v f(v) \cdot \overline{g(v)}.$$

Therefore every bounded operator on it can be represented as a matrix indexed by ordered pairs of vertices of K . Since both Laplacians are bounded operators, the corresponding heat semigroups $e^{-t\Delta}$ and $e^{-t\Delta_\sigma}$ are unambiguously defined for $t > 0$. Let $p_t(v, w)$ and $p_t^\sigma(v, w)$ be the corresponding kernels, i.e. matrices.

We have the following domination relation.

THEOREM 1.5. *For every multiplier σ and every $f \in C_{(2)}^0(K)$ we have*

$$(3) \quad |e^{-t\Delta_\sigma} f| \leq e^{-t\Delta} |f|$$

pointwise. As a consequence,

$$|(e^{-t\Delta_\sigma} f, g)| \leq (e^{-t\Delta} |f|, |g|)$$

for all $f, g \in C_{(2)}^0(K)$. In particular,

$$p_t^\sigma(v, v) \leq p_t(v, v)$$

for every vertex v of K and every $t > 0$.

PROOF. It follows from the inequality in Lemma 1.2 that for every $\lambda > 0$

$$|g| \cdot (\Delta + \lambda I)|g| \leq \Re((\Delta_\sigma + \lambda I)g \cdot \bar{g}) \leq |(\Delta_\sigma + \lambda I)g| \cdot |g|$$

for all $g \in C_{(2)}^0(K)$. It follows that

$$(\Delta + \lambda I)|g| \leq |(\Delta_\sigma + \lambda I)g|.$$

Strictly speaking we can make this conclusion only for vertices where $g(w) \neq 0$. However, when $g(w) = 0$, the left-hand side is nonpositive by (1) and the left-hand side is trivially nonnegative.

Now let $g = (\Delta_\sigma + \lambda I)^{-1}f$. The last inequality can be rewritten as

$$(\Delta + \lambda I)|(\Delta_\sigma + \lambda I)^{-1}f| \leq |f|.$$

Since $(\Delta + \lambda I)$ is positivity preserving we obtain the (pointwise) inequality

$$(4) \quad |(\Delta_\sigma + \lambda I)^{-1}f| \leq (\Delta + \lambda I)^{-1}|f|.$$

By induction,

$$(5) \quad |(\Delta_\sigma + \lambda I)^{-n}f| \leq (\Delta + \lambda I)^{-n}|f|$$

for every positive integer n . Since $e^{-tA} = \lim_{n \rightarrow \infty} (I + (t/n)A)^{-n}$, we conclude that

$$(6) \quad |e^{-t\Delta_\sigma}f| \leq e^{-t\Delta}|f|.$$

This proves the first inequality in the statement of the theorem. The second inequality follows easily from the definition of the inner product. Finally, the last inequality is obtained by setting $g = f = \delta_v$. \square

REMARK 1.6. It is very easy to see (using the equality $\int_0^\infty e^{-t(x+\lambda)}dt = (x+\lambda)^{-1}$) that the inequality (4) used to prove (3) is actually equivalent to it.

We next define the Novikov-Shubin type invariants for the DML. We now assume that the graph K is equipped with a free action of a discrete group G so that the quotient K/G is finite. If $\{v_1, v_2, \dots, v_m\}$ is a fundamental set of vertices of K and A is a bounded operator on $C_{(2)}^0(K)$ that is in commutant of the projective (G, σ) -action on $C_{(2)}^0(K)$ (cf. [12] for a description of this action), for instance the DML, then the von Neumann trace of A is given by

$$(7) \quad \text{tr}_{G,\sigma}(A) = \sum_{i=1}^m (A\delta_{v_i}, \delta_{v_i}).$$

Let $\theta_{G,\sigma}(t) = \text{tr}_{G,\sigma}(e^{-t\Delta_\sigma})$ denote the von Neumann theta function. Choosing a weakly equivalent multiplier determines a unitarily equivalent operator and the von Neumann trace of the new operator remains the same, therefore $\theta_{G,\sigma}(t) = \theta_{G,[\sigma]}(t)$. Explicit calculations tend to show that the large time asymptotics of $\theta_{G,[\sigma]}(t)$ are of the form $O(t^{-\beta})$ for some $\beta > 0$. This motivates the following definitions of the *Novikov-Shubin type invariants* associated to the DML,

$$(8) \quad \beta(G, [\sigma]) = \sup \{\beta \in \mathbb{R} : \theta_{G,[\sigma]}(t) \text{ is } O(t^{-\beta}) \text{ as } t \rightarrow \infty\} \in [0, \infty].$$

The special case $\beta(G, 0) = \beta(G)$ gives the usual Novikov-Shubin invariants of the Laplacian. Let $\text{growth}(G)$ denote the growth rate (exponent) of balls of large metric balls in the group with respect to a word metric. More precisely,

$$\text{growth}(G) = \lim_{r \rightarrow \infty} \frac{\ln(V(r))}{\ln(r)}$$

where $V(r)$ denotes the volume of a ball of radius r in a word metric. We assume here that the group G is finitely generated with a symmetric, finite set of generators S and the distance of the group element g from the identity is the length of the shortest word in letters from S representing it. The volume is simply the cardinality. We recall the following well known theorem of Varopoulos, cf. [17].

THEOREM 1.7. *Let G be a finitely generated discrete group. Then one has*

$$\beta(G) = \frac{\text{growth}(G)}{2}$$

It follows from (6) that for every $t > 0$ and for every $[\sigma]$, one has

$$(9) \quad \theta_{G,[\sigma]}(t) \leq \theta_{G,0}(t).$$

Therefore one has:

COROLLARY 1.8. *Let G be a finitely generated discrete group and σ a multiplier on G . Then*

$$\beta(G, [\sigma]) \geq \frac{\text{growth}(G)}{2} > 0.$$

That is, there is a positive constant C independent of t such that for all $t \gg 0$, one has

$$\theta_{G,[\sigma]}(t) \leq C t^{-\frac{\text{growth}(G)}{2}}$$

1.1. Determinant of the magnetic Laplacian. It follows therefore from (5) that for every $\lambda > 0$ and every positive integer n

$$(10) \quad \text{tr}_G (\Delta + \lambda I)^{-n} \geq \text{tr}_{G,\sigma} (\Delta_\sigma + \lambda I)^{-n}.$$

PROPOSITION 1.9. *Suppose $\ln \det_G(\Delta) > -\infty$ then $\ln \det_{G,\sigma}(\Delta_\sigma) > -\infty$.*

PROOF. Denote by $F(\lambda)$ and $H(\lambda)$ the spectral density functions of Δ and Δ_σ respectively. Multiplying both operators by a suitable constant we can assume that both have norms bounded by one and their density functions are constant for $\lambda > 1$. We also note that $F(0) = H(0) = 0$ since the graph under consideration is infinite.

Recall that

$$(11) \quad \ln \det_G(\Delta) = \int_{0^+}^1 \ln \lambda \, dF(\lambda)$$

$$(12) \quad \ln \det_{G,\sigma}(\Delta_\sigma) = \int_{0^+}^1 \ln \lambda \, dH(\lambda).$$

We begin by observing that a necessary and sufficient condition for $\int_{0^+}^1 \ln \lambda \, dH(\lambda) > -\infty$ is that $\int_{0^+}^1 (1-\lambda)^{-1} \ln \lambda \, dH(\lambda) > -\infty$. Now, for $0 < x \leq 1$,

$$(13) \quad -\frac{\ln x}{1-x} = \frac{1}{1-x} \int_x^1 \frac{du}{u} = \lim_{n \rightarrow \infty} \sum_{k=1}^n \frac{1}{n-k} \cdot \frac{1}{x+k/(n-k)}.$$

The last term in the sum ought to be interpreted as $1/n$. This is simply a Riemann sum approximation of the integral but we remark that it has been chosen so that the approximation is from below and that passing to the subsequence $n = 2^\ell$ we obtain an approximation of the function $-(\ln x)/(1-x)$ by a sequence of positive functions that is increasing in ℓ . For the remainder of the proof we shall write n for 2^ℓ .

Now

$$(14) \quad \infty > - \int_{0^+}^1 (1-\lambda)^{-1} \ln \lambda \, dF(\lambda) =$$

$$\int_{0^+}^1 \lim_{n \rightarrow \infty} \sum_{k=1}^n \frac{1}{n-k} \cdot \left(\lambda + \frac{k}{n-k} \right)^{-1} dF(\lambda)$$

$$= \lim_{n \rightarrow \infty} \sum_{k=1}^n \frac{1}{n-k} \cdot \text{tr}_G \left(\Delta + \frac{k}{n-k} I \right)^{-1},$$

where we have used the monotone convergence theorem to interchange the limit and integration and the fact that $F(0) = 0$ for the equality

$$\int_{0^+}^1 \left(\lambda + \frac{k}{n-k} \right)^{-1} dF(\lambda) = \text{tr}_G \left(\Delta + \frac{k}{n-k} I \right)^{-1}.$$

By our comparison (10) of the trace of the resolvent for Δ and Δ_σ

$$\sum_{k=1}^n \frac{1}{n-k} \cdot \text{tr}_G \left(\Delta + \frac{k}{n-k} I \right)^{-1} \geq \sum_{k=1}^n \frac{1}{n-k} \cdot \text{tr}_{G,\sigma} \left(\Delta_\sigma + \frac{k}{n-k} I \right)^{-1}$$

$$= \int_{0^+}^1 \sum_{k=1}^n \frac{1}{n-k} \cdot \left(\lambda + \frac{k}{n-k} \right)^{-1} dH(\lambda).$$

The integrands in the last integral form a monotone sequence converging to $-(1-x)^{-1} \ln x$ and by (13) and (14) the integrals are bounded by

$$- \int_{0^+}^1 (1-\lambda)^{-1} \ln \lambda \, dF(\lambda).$$

Applying the monotone convergence theorem again we see that

$$- \int_{0^+}^1 (1-\lambda)^{-1} \ln \lambda \, dH(\lambda) < \infty,$$

so that $\int_{0^+}^1 \ln \lambda \, dG(\lambda) > -\infty$.

□

PROPOSITION 1.10. *Let G be an infinite but finitely generated discrete group and σ a multiplier on G . Then $\ln \det_{G,\sigma}(\Delta_\sigma) > -\infty$.*

PROOF. By the Tauberian theorem in [8], we know that Theorem 1.7 is equivalent to the following: there are positive constants C_1, C_2 such that

$$(15) \quad C_1 \lambda^{\frac{\text{growth}(G)}{2}} \leq F(\lambda) \leq C_2 \lambda^{\frac{\text{growth}(G)}{2}}.$$

Integrating equation (11) by parts, one obtains

$$(16) \quad \ln \det_G(\Delta) = \lim_{\epsilon \rightarrow 0^+} \left\{ (-\log \epsilon)(F(\epsilon) - F(0)) - \int_\epsilon^1 \frac{F(\lambda)}{\lambda} d\lambda \right\}$$

Using the fact that $\liminf_{\epsilon \rightarrow 0^+} (-\log \epsilon)(F(\epsilon) - F(0)) \geq 0$ (in fact, this limit exists and is zero) and $\frac{F(\lambda)}{\lambda} \geq 0$ for $\lambda > 0$, one sees using equation (1.8) that

$$(17) \quad \ln \det_G(\Delta) \geq - \int_{0^+}^1 \frac{F(\lambda)}{\lambda} d\lambda \geq - \frac{2C_2}{\text{growth}(G)} > -\infty.$$

The proof of the Proposition is completed by an application of Proposition 1.9. \square

2. Existence and properties of a ground state

In this section we follow the notation and formalism of [6]. An excellent discussion of analogous questions in the continuous case can be found in [13]. Let K be an infinite, connected graph of bounded valence, i.e. $m(x) \leq M$ for a constant $M > 0$ independent of $x \in K$. We abuse the notation slightly and write K for both the graph and the set of its vertices. The combinatorial Laplacian Δ on K or a subgraph of K acts on functions by the formula (1). Our sign convention makes Δ a nonnegative, self-adjoint operator. Let K_1 be a subgraph of K . We denote by $\overset{o}{K}_1$ the set of vertices of K_1 all of whose neighbors are in K_1 . ∂K_1 is the complement of $\overset{o}{K}_1$ in K_1 .

The following elementary lemmata have been proved in [6].

LEMMA 2.1. *Suppose $u(x)$ is a real-valued function on K_1 and $x \in \overset{o}{K}_1$. If $\Delta u(x) < 0$, then u does not have a maximum at x .*

LEMMA 2.2. *Suppose $u(x)$ is a function on K_1 and $u > 0$, $\Delta u > 0$ on $\overset{o}{K}_1$. If $x \sim y$ and both x and y are in $\overset{o}{K}_1$, then*

$$\frac{1}{m(y)} \leq \frac{u(y)}{u(x)} \leq m(x).$$

In the sequel, we refer to Lemma 2.1 and Lemma 2.2 as the maximum principle and the Harnack inequality respectively.

Using these lemmata we prove the existence of a ground state.

THEOREM 2.3. *Let $\lambda_0 = \inf \text{spec } \Delta$. There is a positive eigenfunction ϕ of Δ on K belonging to λ_0 , i.e.*

$$\Delta\phi = \lambda_0\phi, \quad \phi > 0.$$

REMARK 2.4. ϕ need not be square-summable. The cone of such functions need not be one dimensional in general. We do not know whether ϕ is necessarily bounded under our assumption on K .

PROOF. Consider an exhaustion K_n of K by an increasing sequence of finite subgraphs K_n such that $\overset{\circ}{K_n} \subset K_{n+1}$. On each K_n consider the combinatorial Laplacian Δ_n acting on functions that vanish on the boundary of K_n . Call λ_n the smallest eigenvalue of the combinatorial Laplacian Δ_n . By [6], $\lambda_n > \lambda_0 \geq 0$ and λ_n converges to λ_0 . Let ϕ_n be the eigenfunction of Δ_n belonging to λ_n normalized so that $0 < \phi_n$ inside K_n and $\phi_n(x_0) = 1$ for some fixed point x_0 that belongs to all K_n . Note that $\Delta\phi_n(x) = \lambda_n\phi_n(x) > 0$ in the interior of K_n . Since $\phi_n(x_0) = 1$, it follows now from the Harnack inequality and the connectedness of K that the sequence $\phi_n(x)$ is bounded for every fixed $x \in K$. Using the diagonal process we choose a subsequence, still denoted ϕ_n that converges at *all* points of K . Let ϕ be the limit of this subsequence. Since $\lim_{n \rightarrow \infty} \phi_n = \phi$ and $\lim_{n \rightarrow \infty} \lambda_n = \lambda_0$

$$\Delta\phi = \lambda_0\phi.$$

The limit function ϕ satisfies $\phi \geq 0$, $\phi(x_0) = 1$. It is strictly positive by the maximum principle applied to $-\phi$. \square

Note that the ground state ϕ constructed above can be identically equal to one if $\lambda_0 = 0$. However, in the nonamenable case, $\lambda_0 > 0$ and ϕ is nonconstant.

We denote by $d(x, y)$ the distance between x and y in K i.e. the length of shortest chain of edges connecting x with y . The following lemma is an easy consequence of the Harnack inequality.

LEMMA 2.5. *If ϕ is the ground state constructed above so that $\phi(x_0) = 1$ then, for all $x \in K$, ϕ satisfies*

$$M^{-d(x, x_0)} \leq \phi(x) \leq M^{d(x, x_0)},$$

where M is the uniform bound on the valence of vertices of K .

From now on we refer to the normalized ground state ϕ as above as the ground state.

To prove a further property of the ground state ϕ (so called completeness) we investigate its behavior under the heat semigroup. Since the combinatorial Laplacian is a bounded operator on $C_2^0(K)$, $\|\Delta\| \leq 2\sqrt{M}$ with our definition of the inner product, $e^{-t\Delta}$ is defined unambiguously as

$$(18) \quad P_t = e^{-t\Delta} = \sum_{n=0}^{\infty} \frac{(-t)^n \Delta^n}{n!}.$$

Its kernel (matrix) is given by

$$p_t(x, y) = (P_t \delta_x, \delta_y).$$

We need to estimate the behavior of $p_t(x, y)$ for bounded t and large $d(x, y)$.

LEMMA 2.6. *For every $T > 0$ there exist a constant $C(T) > 0$ such that*

$$p_t(x, y) \leq \frac{C}{d(x, y)!}$$

for all $t \in [0, T]$.

PROOF. Write $\Delta^n(x, y)$ for the matrix coefficient of the n -th power of Δ . Then $\Delta(x, y) = 0$ if $d(x, y) > 1$ by the definition of the combinatorial Laplacian. It follows, that $\Delta^n(x, y) = 0$ if $d(x, y) > n$. Now suppose that $d(x, y) = m$. It follows from (18) that

$$(19) \quad p_t(x, y) = \sum_{n=m}^{\infty} \frac{(-t)^n \Delta^n}{n!}.$$

Since the combinatorial Laplacian is bounded,

$$|\Delta^n(x, y)| = |(\Delta^n \delta_x, \delta_y)| \leq c^n.$$

Therefore the series obtain by factoring out $1/m!$ from (19) is easily seen to be uniformly bounded for $t \leq T$. This proves the lemma. \square

In view of the decay estimate above, the heat semigroup originally defined on square-summable functions can be extended to functions of moderate growth at infinity. Formally,

$$P_t u(x) = \sum_{y \in K} p_t(x, y) u(y).$$

For example, since the number of vertices of K grows exponentially with distance as does the ground state ϕ the series

$$P_t \phi(x) = \sum_{y \in K} p_t(x, y) \phi(y)$$

converges very rapidly. Our goal is to prove that the ground state ϕ is complete in the sense that

$$(20) \quad e^{-\lambda_0 t} P_t \phi(x) = \phi(x).$$

To place this in a proper context, consider the renormalized semigroup

$$\tilde{P}_t = e^{\lambda_0 t} [\phi^{-1}] P_t [\phi],$$

where $[u]$ denotes the operator of multiplication by the function u . The infinitesimal generator $\frac{d}{dt}|_{t=0} \tilde{P}_t$ is equal to $-[\phi^{-1}](\Delta - \lambda_0)[\phi] = -L$. A calculation shows that

$$(21) \quad Lu(x) = \sum_{y \sim x} \frac{\phi(y)}{\phi(x)} (u(x) - u(y)).$$

In order to prove (20) we study bounded solutions of the initial value problem

$$(22) \quad \begin{aligned} Lu + \frac{\partial u}{\partial t} &= 0 \\ u(x, 0) &= u_0(x) \end{aligned}$$

using the method of [7].

We need the parabolic version of the maximum principle.

LEMMA 2.7. *Suppose $u(x, t)$ satisfies the inequality $Lu + \frac{\partial u}{\partial t} < 0$ on $\overset{\circ}{K}_1 \times [0, T]$. Then the maximum of u on $K_1 \times [0, T]$ is attained on the set $K_1 \times \{0\} \cup \partial K_1 \times [0, T]$.*

PROOF. Suppose $(x_0, t_0) \in \overset{\circ}{K}_1 \times (0, T]$ is a maximum. It follows that $\frac{\partial u}{\partial t}(x_0, t_0) \geq 0$ so that $Lu(x_0, t_0) < 0$. On the other hand, (21) and positivity of ϕ imply that $Lu(x_0, t_0) \geq 0$. The contradiction proves the lemma. \square

We now state and prove the main result of this section.

THEOREM 2.8. *Let $u_0(x)$ be a bounded function on K , $|u_0(x)| \leq N_0$. Then the initial value problem (22) has a unique bounded solution $u(x, t)$. In addition,*

$$|u(x, t)| \leq |N_0|$$

for all (x, t) .

PROOF. In view of the remarks above about the decay of $p_t(x, y)$

$$u(x, t) = \tilde{P}_t u_0(x) = \sum_{y \in K} e^{\lambda_0 t} p_t(x, y) \frac{\phi(y)}{\phi(x)} u(y)$$

is defined by a rapidly converging series and formal calculations showing that it satisfies (22) are justified. This gives existence. Now suppose that $u(x, t)$ is a bounded solution. Let $N_1 = \sup |u(x, t)|$. Fix $x_0 \in K$ and define $r(x) = d(x, x_0)$. By our assumption on the valence and the Harnack inequality

$$(23) \quad |Lr| < M^2.$$

Consider an auxiliary function

$$v(x, t) = u(x, t) - N_0 - \frac{N_1}{R}(r(x) + M^2 t),$$

where R is a large parameter. Let $K_1 = B(x_0, R)$ be the set of vertices of K at distance at most R from x_0 . The function $v(x, t)$ is nonpositive on the set $K_1 \times \{0\} \cup \partial K_1 \times [0, T]$ and satisfies $(Lu + \frac{\partial}{\partial t})u < 0$ on $\overset{\circ}{K}_1 \times [0, T]$ because of (23). Lemma 2.7 implies therefore that $v(x, t) \leq 0$ so that

$$u(x, t) \leq N_0 + \frac{N_1}{R}(r(x) + Mt)$$

on $B(x_0, R) \times [0, T]$. Keeping (x, t) fixed and letting R increase without bounds, we see that $u(x, t) \leq N_0$. Applying the same argument to $-u$ yields $|u(x, t)| \leq N_0$. Since $T > 0$ and x were arbitrary, this last inequality holds for all $x \in K$ and $t \geq 0$. Uniqueness follows by considering the difference of two solutions. \square

COROLLARY 2.9. *The ground state ϕ is complete, i.e.*

$$e^{\lambda_0 t} \sum_{y \in K} p_t(x, y) \phi(y) = \phi(x)$$

for all $x \in K$ and $t > 0$.

PROOF. The function $u(x, t)$ identically equal to one satisfies the initial value problem (22) with the initial value $u_0(x)$ identically one. $\tilde{P}_t u_0(x)$ is another solution with the same initial value. The two must be equal. Hence

$$e^{\lambda_0 t} \sum_{y \in K} p_t(x, y) \frac{\phi(y)}{\phi(x)} = 1$$

for all $x \in K$ and $t \geq 0$. □

We remark that Lemma 2.7 and Theorem 2.8 hold for the Laplacian Δ as well as for the renormalized Laplacian L since both the maximum principle and the Harnack inequality hold for Δ . This implies that the fundamental solution $p_t(x, y)$ for the heat equation on the graph K of bounded valence is unique since it is a bounded solution of the initial value problem

$$(24) \quad \begin{aligned} \Delta u + \frac{\partial u}{\partial t} &= 0 \\ u(x, 0) &= \delta_y. \end{aligned}$$

This fact is of independent interest and we state it separately as

THEOREM 2.10. *For a graph K of bounded valence, the fundamental solution of the heat equation is unique. More precisely, the function $p_t(x, y)$ of variables $t \geq 0$ and $x, y \in K$ is the unique bounded, positive solution $v(x, y, t)$ of the equation $\Delta_x v + \frac{\partial v}{\partial t} = 0$ satisfying the initial condition $v(x, y, 0) = \delta_y(x)$.*

3. Long time decay of the heat kernel

We now give a discrete analog of a proof, due to Terry Lyons in the continuous case, of the decay of $p_t(x, x)$ as $t \rightarrow \infty$. Recall that the graph K is equipped with a free action of a discrete group G and the quotient K/G is finite. If $\{v_1, v_2, \dots, v_m\}$ is a fundamental set of vertices of K and A is a bounded operator on $\ell^2(K)$ that is in commutant of the G action on K , for instance the combinatorial Laplacian, then the von Neumann trace of A is given by

$$\text{tr}_G(A) = \sum_{i=1}^m (A\delta_{v_i}, \delta_{v_i}).$$

Let $\theta_G(t) = \text{tr}_G(e^{-t\Delta})$ denote the von Neumann theta function. Define

$$(25) \quad \beta(K) = \sup \left\{ \beta \in \mathbb{R} : e^{t\lambda_0(K)} \theta_G(t) \text{ is } O(t^{-\beta}) \text{ as } t \rightarrow \infty \right\}.$$

The continuous analog of the proposition below is contained in the Appendix to [5]. Our proof is patterned after the argument there.

PROPOSITION 3.1. *Under the assumptions above, $\theta_G(t) \leq Ce^{-\lambda_0 t}t^{-1}$ for large t . In particular, $\beta(K) \geq 1$.*

PROOF. If $\lambda_0 = \lambda_0(K) = 0$ the statement follows from Theorem 1.7 so we assume that $\lambda_0 > 0$ from now on. Recall that this implies that the group G is nonamenable. By the Theorem 2.3, there is a ground state, that is, a $\phi > 0$ such that $\Delta\phi = \lambda_0\phi$. Then either there is a $\gamma \in G$ such that $\gamma^*\phi$ is not proportional to ϕ , or for every $\gamma \in G$,

$$\gamma^*\phi = \alpha(\gamma)\phi$$

for some morphism $\alpha : G \rightarrow \mathbb{R}_+$.

Case 1. Suppose that there is a $\gamma \in G$ such that $\gamma^*\phi$ is not proportional to ϕ . Then

$$u = \frac{\gamma^*\phi}{\phi} > 0$$

is a positive, non-constant harmonic function for the Markovian semi-group with matrix

$$\tilde{p}_t(x, y) = e^{\lambda_0 t} p_t(x, y) \frac{\phi(y)}{\phi(x)}.$$

This can be seen as follows. A simple calculation using the G invariance $p_t(x, y) = p_t(\gamma x, \gamma y)$ of the heat kernel yields

$$\tilde{P}_t u(x) = e^{\lambda_0 t} \phi(x)^{-1} \sum_{y \in K} p_t(\gamma x, y) \phi(y)$$

which, by Lemma 2.9, is equal to $\frac{\phi(\gamma x)}{\phi(x)} = u(x)$.

Case 2. Suppose that for every $\gamma \in G$,

$$\gamma^*\phi = \alpha(\gamma)\phi$$

for some morphism $\alpha : G \rightarrow \mathbb{R}_+$. Then the Markovian semigroup

$$\tilde{p}_t(x, y) = e^{\lambda_0 t} p_t(x, y) \frac{\phi(y)}{\phi(x)}$$

is G invariant, by a simple calculation. Now by [11], Theorem 3 and the comment at the end of Section 5 of [11], \tilde{p}_t admits a non-constant, positive, harmonic function u .

Thus in both cases, $\tilde{p}_t(x, y)$ admits a positive, nonconstant, harmonic function. We use this fact to prove the finiteness of the integral $\int_1^\infty e^{\lambda_0 t} p_t(x, x) dt$ as follows. Observe that

$$e^{\lambda_0 t} p_t(x, x) = (e^{-t(\Delta - \lambda_0)} \delta_x, \delta_x).$$

It follows that the function $t \rightarrow e^{\lambda_0 t} p_t(x, x)$ is non-increasing. Therefore the convergence of the integral $\int_1^\infty e^{\lambda_0 t} p_t(x, x) dt$ is equivalent to the convergence of the sum $\sum_{n=1}^\infty e^{\lambda_0 n} p_n(x, x)$.

Now the restriction of $\tilde{p}_t(x, y)$ to positive integer values of t defines a Markov chain with transition probabilities $q_n(x, y) = \tilde{p}_n(x, y)$. Clearly, the functions harmonic for $\tilde{p}_t(x, y)$ are harmonic for $q_n(x, y)$. By [10, Proposition 6.3, Chapter 6] this Markov chain is transient, i.e.

$$\sum_{n=1}^{\infty} q_n(x, x) = \sum_{n=1}^{\infty} e^{\lambda_0 n} p_n(x, x)$$

is finite. Thus $\int_1^{\infty} e^{\lambda_0 t} p_t(x, x) dt < C$ and, using the monotonicity again, we obtain

$$\frac{t}{2} e^{\lambda_0 t} p_t(x, x) \leq \int_{t/2}^t e^{\lambda_0 s} p_s(x, x) ds \leq C'.$$

Summation over x in a fundamental domain yields $\theta_G(t) = O(e^{-\lambda_0 t} t^{-1})$.

□

Proposition 9 gives an estimate for the trace of the heat kernel of the discrete Laplacian. An analogous estimate holds for the magnetic Laplacian. More precisely, we have:

COROLLARY 3.2. *For every multiplier σ ,*

$$e^{\lambda_0(K)t} \operatorname{tr}_{G,\sigma}(e^{-t\Delta_\sigma}) = O(t^{-1})$$

for large t . In addition, if T is a bounded operator on $C_{(2)}^0(K)$ that commutes with the projective (G, σ) -action, and satisfies $T \geq -\lambda_0(K)$, then

$$\operatorname{tr}_{G,\sigma}(e^{-t(\Delta_\sigma+T)}) = O(t^{-1}).$$

PROOF. The first inequality follows from the discrete Kato inequality,

$$\operatorname{tr}_{G,\sigma}(e^{-t\Delta_\sigma}) \leq \operatorname{tr}_G(e^{-t\Delta})$$

and Proposition 3.1. The second inequality is a consequence of the first one in view of [9, Theorem 2.16]. □

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PH.D. PROGRAM IN MATHEMATICS, GRADUATE CENTER OF CUNY, NEW YORK, NY 10016, USA.
E-mail address: jozek@derham.math.qc.edu

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF ADELAIDE, ADELAIDE 5005, AUSTRALIA
E-mail address: vmathai@maths.adelaide.edu.au